Network Attributes Impacting the Generation and Flow of Knowledge Within and From the Basic Science Community

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Partial Theoretical Framework

- Collective and Dynamic Nature of Science – the "invisible college"(Polanyi) – organizes itself around problems
- Knowledge Leveraged Through Sharing and Combination (Shumpeter) – Importance of the Community/Network
- Science Advanced in An Ecology of Dynamic and Overlapping Communities
- Close Relationship (co-evolutionary) – between Social, Human and Intellectual Capital
- Importance of Application (Stokes) – Dynamic Interplay Between Advancing of Science and Application

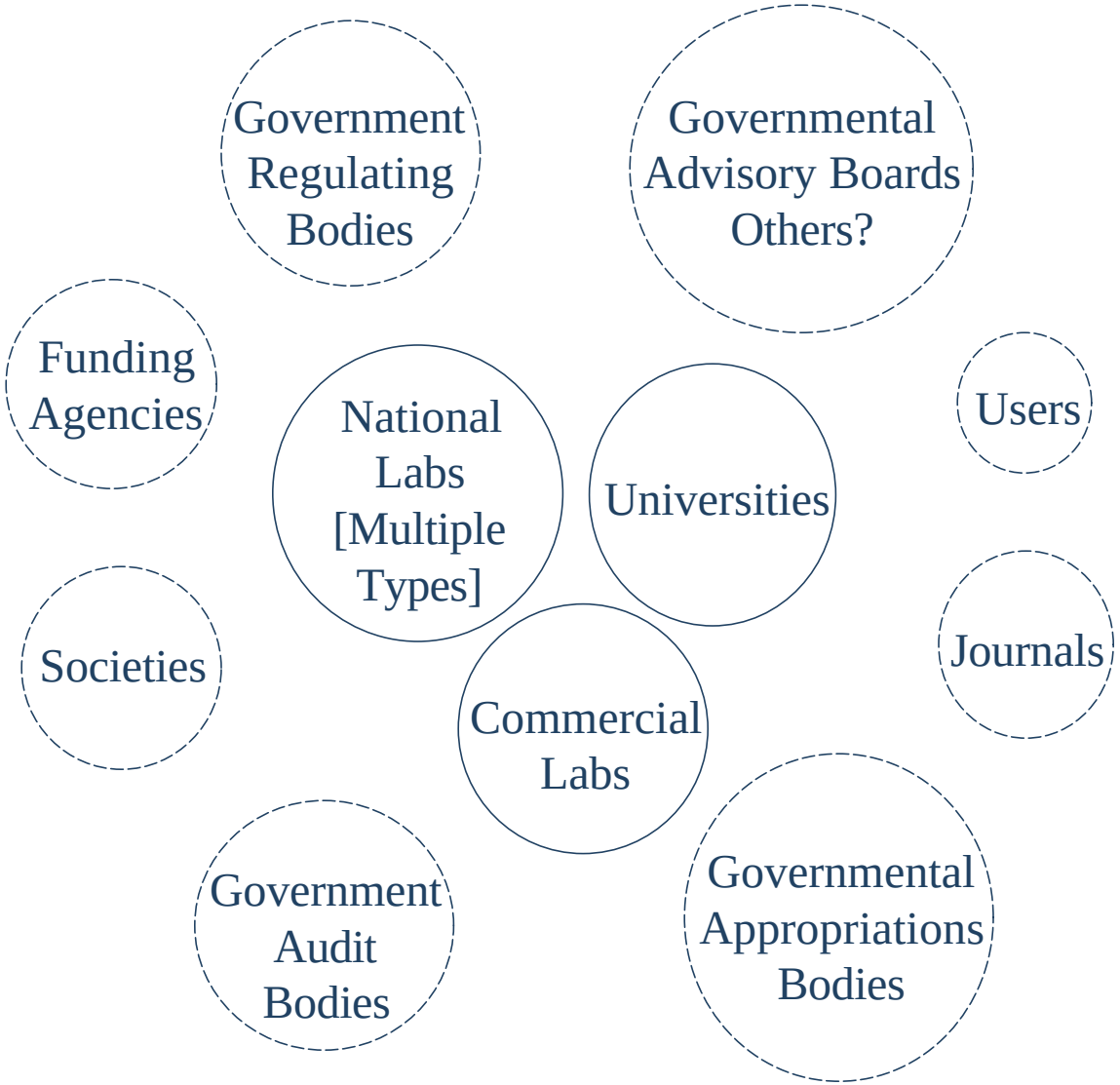
Partial Theoretical Framework

- **Importance of Organization (although "invisible")**
  - **Modern Science - scale, technology and information processing requirements**
  - **Organizational skill required to do complex sets of interrelated research steps and projects**
- **Not a Traditional Hierarchical Organization**
  - **Stress importance of:**
    - **Freedom to explore and move out of confines of discipline and stated problem**
    - **Coordination around problem, not objectives**
  - **Self-organizing**
    - **Doesn't take place in one institutional or organizational setting**

Definition of Value/Outcomes

- **Based on DOE conference on outcomes - focusing on knowledge as the key outcome of basic research.**
  - **In the context of Applied Math:**
    - **1) Algorithms, theorems that become embodied in:**
      - **a) articles, presentations**
      - **b) code**
    - **2) SW products (enabling technology):**
      - **code**
      - **libraries**
      - **frameworks**
    - **3) These products and enabling technology can be:**
      - **generic mathematical approaches**
      - **customized/incorporated into different applications domains**
- **We are systematically tracking the knowledge outcomes and how they flow.**

The Network Elements (Organizational)



Research Questions

- **What approaches to modeling the network are useful for displaying and analyzing the flow of value within and from the network?**
- **What are the attributes of the research network that facilitate the flow (leverage) of "value" through the network?**
- **What organizational features facilitate these forms of network?**

Methodology/Data Collection

- **Qualitative Interview Data Re:**
  - **History of /Activities in the Network**
  - **Nature of Collaborations**
  - **Organizational Features**
- **Survey/Network Grid Completion Re:**
  - **Collaborations**
  - **Sources of Knowledge**
  - **Value of Knowledge Flowing Through Links**
- **Archival (CV) Analysis for Demographic Attributes**

Methodology / Analysis

- Network Depiction and Measurement
- Qualitative Case Analysis
- Multivariate Analysis

Sandia MPP / Modeling and Simulation Enabling Technology

First Test Adopters	Early Adopters	Wide–spread Adoption	MPP as a Tool – Focus on capability development
Phase 1: 1986-1992	**Phase 2: 1992-1996**	**Phase 3: 1996-2001**	**Phase 4: 2000** →
"Proof of Concept"	Algorithmic/Capability Development (MPSalsa)	→ Continues	Integration of Code
Early linear solvers algorithms & codes	Reacting Flow Simulations "Test-Bed" Code	→ Continues	→ Continues
	"Branch" Codes build on MPSalsa for other applications	"Ripening" of Codes Spin off libraries and frameworks	→ Continues
		Capabilities incorporated into many applications	→ Continues
			New mathematical / algorithmic development for bigger and more complex problems

Phase 1 – 1986-1992
Early Work with Linear Solvers on MPP

Algorithmic Development / Generalizable Mathematics / Enabling Technologies

LDRC
CSRF
MICS

Some theory on and demonstration of Parallel multi-level methods:
- Dense linear solvers
- Parallelizing multi-grid
- General iterative methods

MICS

- Develop MP iterative Krylov solvers for structured meshes
- Develop MP preconditioners:
  - algebraic
  - multilevel

- Early Load-Balancing Work

MPSalsa

Related Development & Applications

CSRF

- Iterative solvers in Coyote FE code using early version of Aztec (Krysolve)

Further Dissemination

- First Gordon Bell Winner

Phase 2 – 1992-1996
Reacting Flow Simulations / Generalize linear Solvers

Algorithmic Development / Generalizable Mathematics / Enabling Technologies
- **Non-Linear Solvers**
- **Static Load Balancing**
- **Optimization**

MICS
CSRF LDRD
- Extend MP Krylov solvers for unstructured meshes
- Develop MP preconditioners:
  - algebraic
- Develop Aztec library

MICS
- Graph partitioning
- Chaco 1.0

MICS
CSRF LDRD
ASCI
- Develop domain decomposition preconditioners
- Develop incomplete factorization subdomain preconditioners
- Release Aztec 1.0 Library

MICS
- Graph partitioning enhancements
- Chaco 2.0

FFT's in parallel materials modeling

- Algorithms for Parallel Particle Simulations

MPSalsa: Implicit FE technique / unstructured mesh problems

CSRF LDRD
- Develop 2D/3D GLS laminar reacting flow formulation
- Develop MP FE kernals
- Develop MP FE ExodusII databases (Nemesis)

MICS
- Develop fully-coupled laminar chemically reacting flow solvers
- Develop inexact Newton solvers
- Develop block sparse FE formulation

CSRF LDRD
ASCI
- Develop MP turbulent chemically reacting flow code (combustion, catalysis)
- Develop high Re GLS implementation
- Develop LES/LEM implementation
- In adaptivity
- MPSalsa 1.0

Related Development & Applications

- Seismic Imaging

ESRF
- GOMA development using MPSalsa infrastructure

MICS
- CVD modeling SiN4, SiC, GaAs
- CVD optimization prototyping

ESRF LDRD
- MP Multiphase flow development based on MPSalsa infrastructure

ASCI
- Alegra

- PorSalsa

- Finite Difference Code

- CTH - parallel shock physics

Further Dissemination

- 1994 MPSalsa Gordon Bell
- Competition Finalist

- Winner Gordon Bell Award-dense linear solvers

- Publish papers

- R&D 100 '94

- Begin external collaborations on reacting flow simulations

- Begin dissemination to ASCI
- Effort, Algorithms/Software/consulting

Phase 3 – 1996-2001

• Continuation of development of parallel implicit finite and linear solver element methods

• Salsa releases incorporating advanced solver algorithms, turbulent flow, optimization, bifurcation

Algorithmic Development / Generalizable Mathematics / Enabling Technologies

- Parallel data processing
- Adaptivity
- Optimization
- Advanced solver algorithms

MICS
ASCI

- Develop matrix-free interface
- Develop multilevel library / application interface definition
- Develop multilevel preconditioners
- Domain Decomp.

MICS
ASCI

- Aztec 1.1, 2.0, and 2.1
  - Parallel solver library
- Nonlinear Solver work

Tightly coupled optimization
RSQP++
Dakota

CSRF
MICS

- LOCA:
  - Continuation bifurcation stability analysis
  - Methods/Library

MICS
ASCI

- ARPACK
  - Eigen system analysis
- Anasazi
- Multi-Level

MICS
ASCI

- Zoltan:
  - Dynamic load balancing
  - Methods/ Library

MICS

- Early work on Trilinos
- Object oriented solver framework

Nemesis: MPP FE database software

Algorithms for Parallel Crash Simulations - PRONTO

Adaptivity

Parallel FFT's

MPSalsa: Parallel implicit finite elements and solution algorithms

CSRF LDRD

Incorporation of:
- Advanced solver algorithms
- Turbulent flow
- Optimization
- Bifurcation

→ MPSalsa 1.5

Related Development & Applications

ASCI and other application codes:
- Legacy codes
- Parallelized
- Zyce

TRS Systems:
- Simulation oriented to turbulent flow
- Physics engineering applications

- Plasma and semiconductor
- Modeling exploration with Stab. FEM

Application

New Engineering Mechanics Codes:
- Thermal
- Fluid
- Structural

- Tramonto Code
  Biology, materials & nano-technology
- Alegra
  Interface to Aztec
- Catalysts
- Nimrod
- Zapotec

Further Dissemination

- Continued Impact on ASCI
- Algorithms/Software /Consulting

- Publish papers/invited talks

- Continued ext. collab.
- '99 Seismic Imaging R&D 100 Award

- 1997 Aztec R&D100 Award
- 1997 MPSalsa Gordon Bell Finalist

Phase 4 – 2001 on

Algorithmic Development / Generalizable Mathematics / Enabling Technologies

ASCI
- Aztec '00

MICS
ASCI
- Trilinos Evolution
  - NOX-Non Linear solver package
  - Interoperability

Support Theory
Graph Based Preconditioning

MICS
- Theoretical work on stabilized FE methods for PDE's

Parallel Adaptivity

MICS
ASCI

Unstructured mesh/complex physics:
- ML solver package and preconditioners
- AMG and physics-based preconditioners
- Prometheus
- Anasazi

- 2-Level domain decomposition
- Block approximation factorizations & AMG
- Belos, Meros

Non-linear operator splitting and time discretizations

On-going work on:
- Dynamic load balancing
- Continuation, bifurcation (LOCA)

Krylov Methods for time integration

Moocho (optimization)

Adaptive Multi-Grid

Multi-Scale

Continuum Modeling

Discretization Algorithms

MPSalsa: Transport Reaction Systems

- Parallel FE with transport reaction simulation capability
- Development of preconditioners

Athena → Olympus

Related Development & Applications

ASCI

Allegra Multi
H Curl Magnetic Solution Technologies
Maxwell Multi-Grid

ASCI
- Electrical Modeling & Simulation
- Sierra/Promo User NDX

MICS
Other SANDIA contracts
- Cell biology
- Fuel cells

- Chem/bio simulations

- Charon: Semiconductor
- Device Modeling Code
- Zyce

LES (Large Eddy Simulations)

SW Quality / SQA Standards

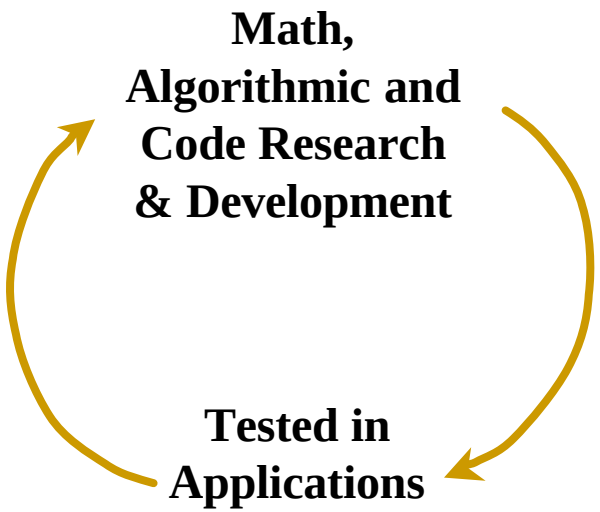
LDRD/CRADA
- Solid State Lighting

FEI
- Sierra
  - Fuego
  - Adagio
  - Presto
  - Salinas
  - Aria
- CLLML
  - ALE3D
  - CLLML

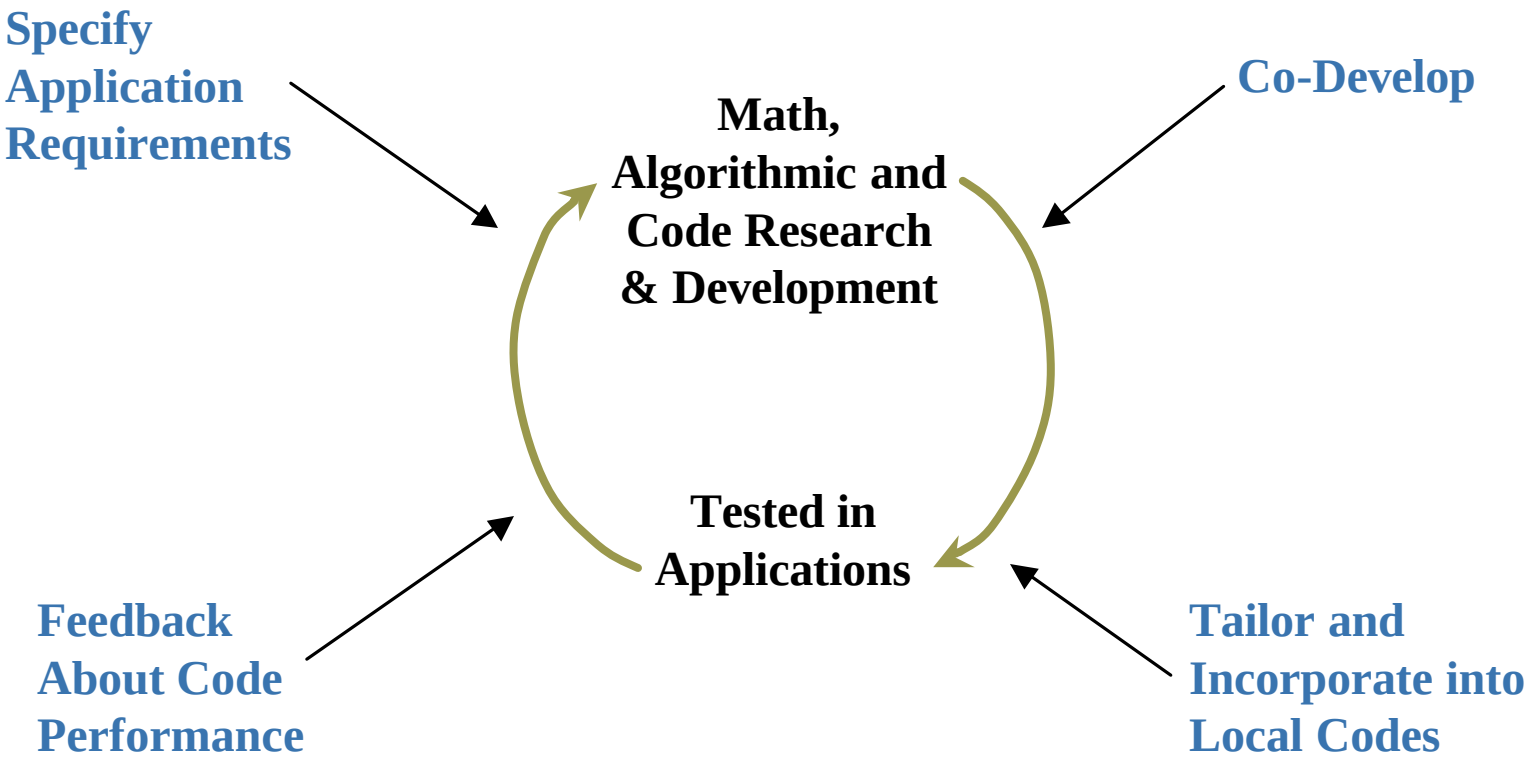
Further Dissemination

Continued impact of ASCI, ext. collab, papers, invited talks, mini-symposia

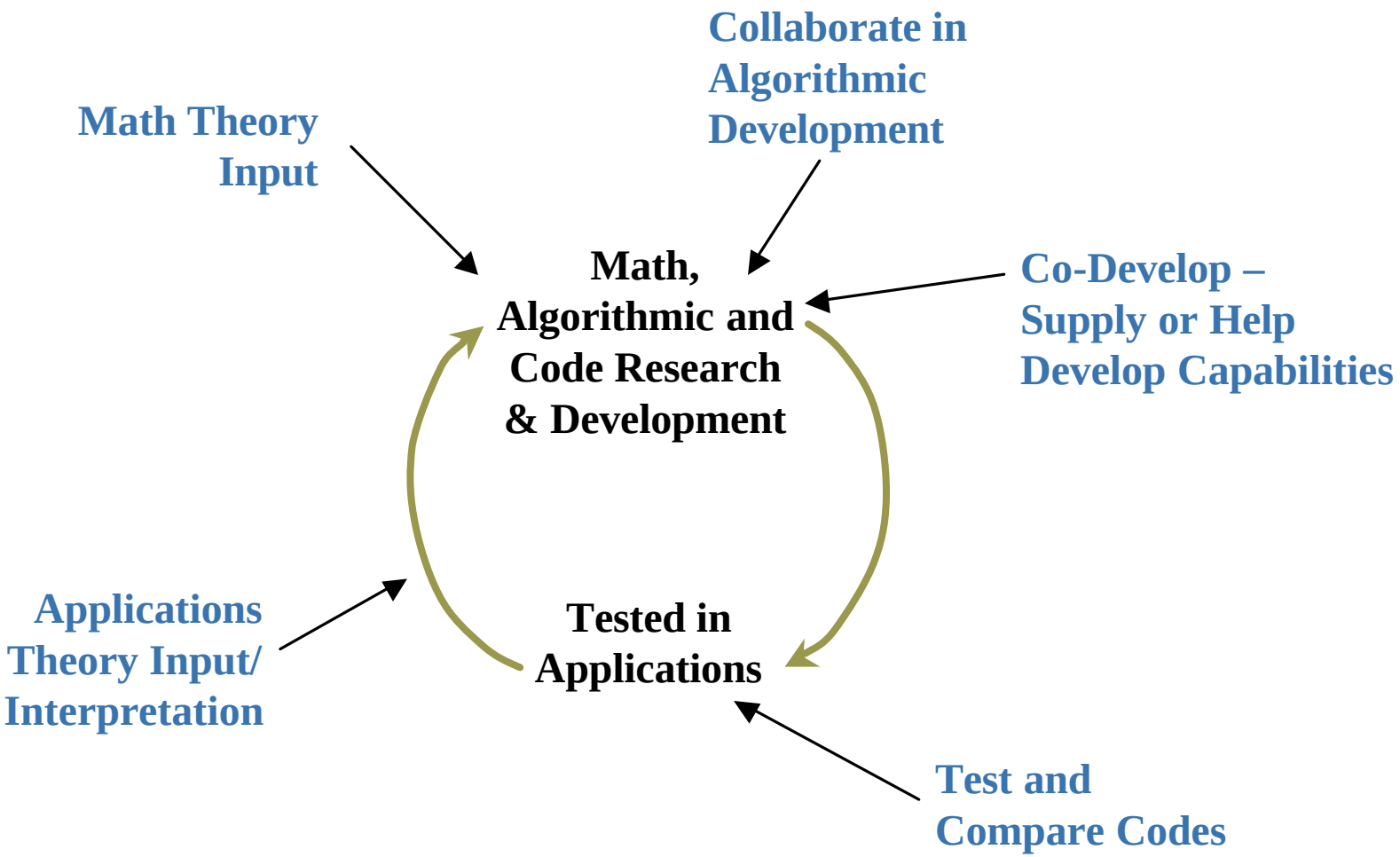
Cycle of Learning



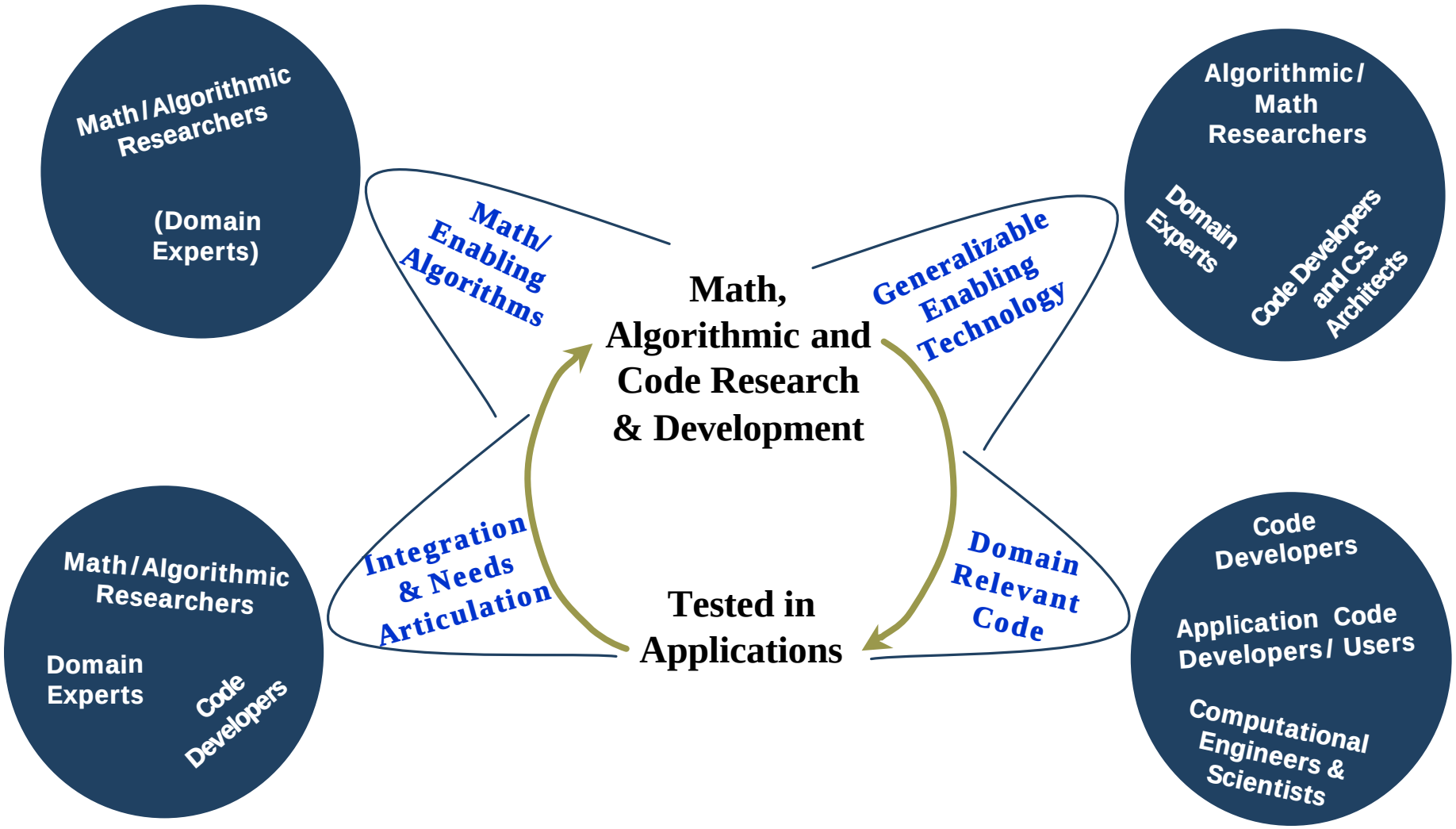
Cycle of Learning: Roles of Applications Collaborators



Cycle of Learning: Roles of Academic /External Collaborators

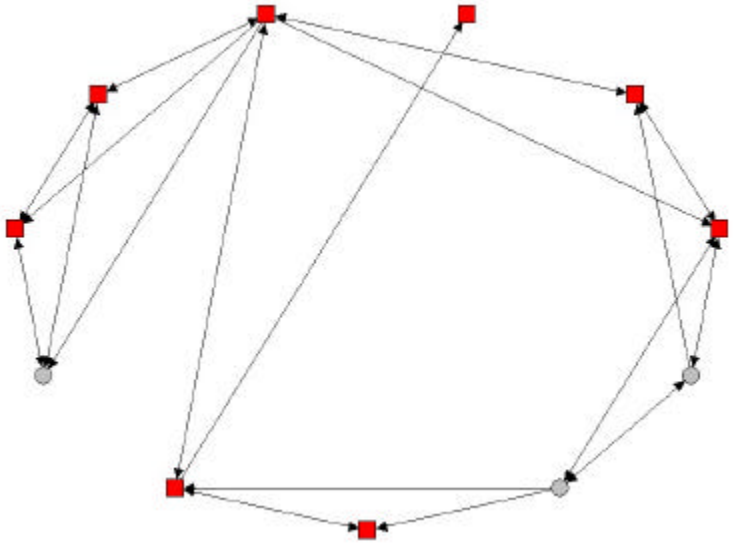


Cycle of Learning: Examples of Sub-Networks



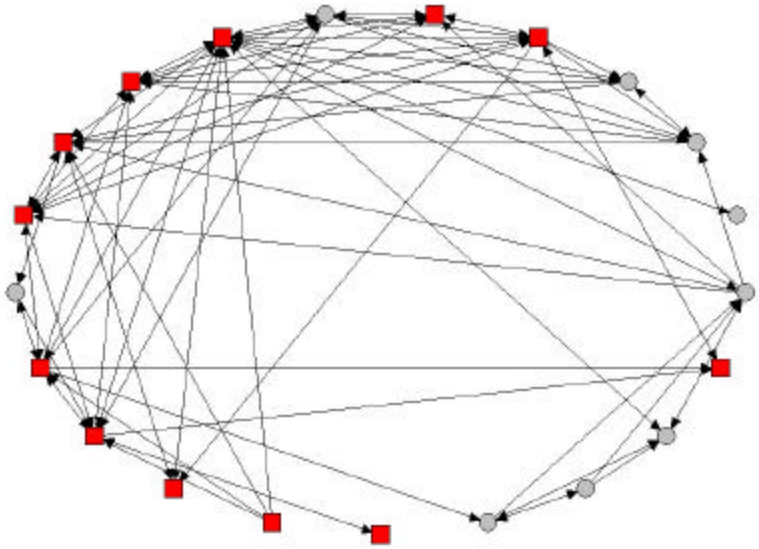
Collaboration MICS – Phase 1

Red squares = MICS funding; Gray Circles= no MICS



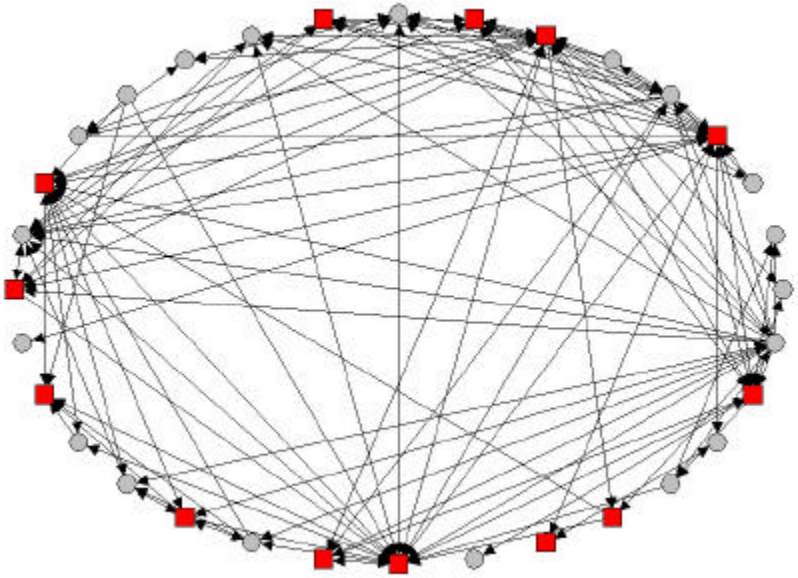
Collaboration MICS – Phase 2

Red squares = MICS funding; Gray Circles= no MICS



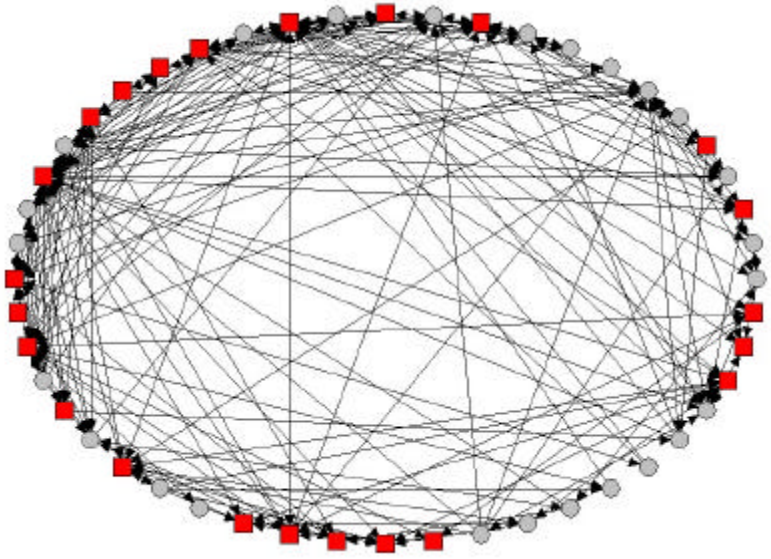
Collaboration MICS – Phase 3

Red squares = MICS funding; Gray Circles= no MICS



Collaboration MICS – Phase 4

Red squares = MICS funding; Gray Circles= no MICS



Collaboration Density: MICS versus Non-MICS Funding

Phase 1

Interviewees \ Members	MICS	Non-MICS
MICS	.2679	.2083
Non-MICS	.2917	.3333

Phase 2

Interviewees \ Members	MICS	Non-MICS
MICS	.3788	.1481
Non-MICS	.1667	.1944

Phase 3

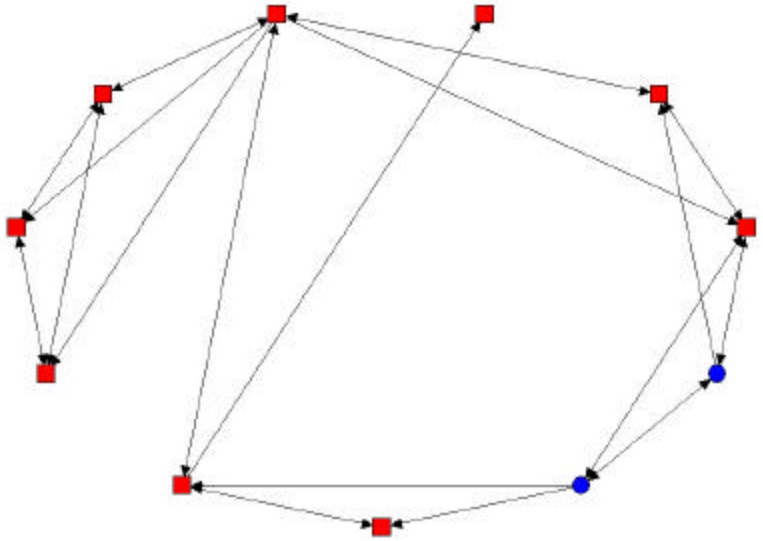
Interviewees \ Members	MICS	Non-MICS
MICS	.3333	.1377
Non-MICS	.2186	.0819

Phase 4

Interviewees \ Members	MICS	Non-MICS
MICS	.1932	.1183
Non-MICS	.1323	.0667

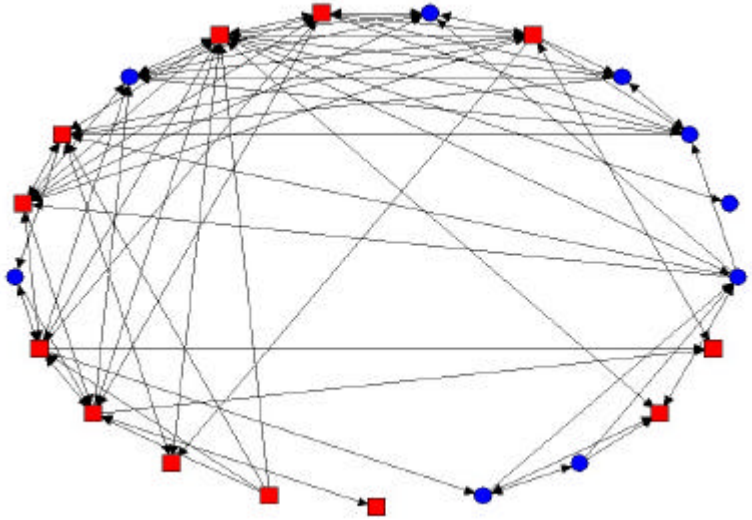
Collaboration ROLES - PHASE 1

Red squares=Math/Computer Sciences; Blue Circles=Applications



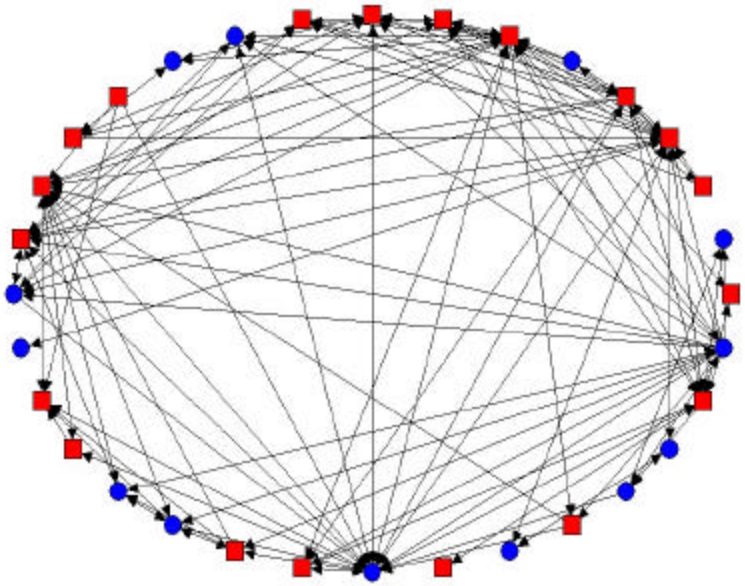
Collaboration ROLES - PHASE 2

Red squares=Math/Computer Sciences; Blue Circles=Applications



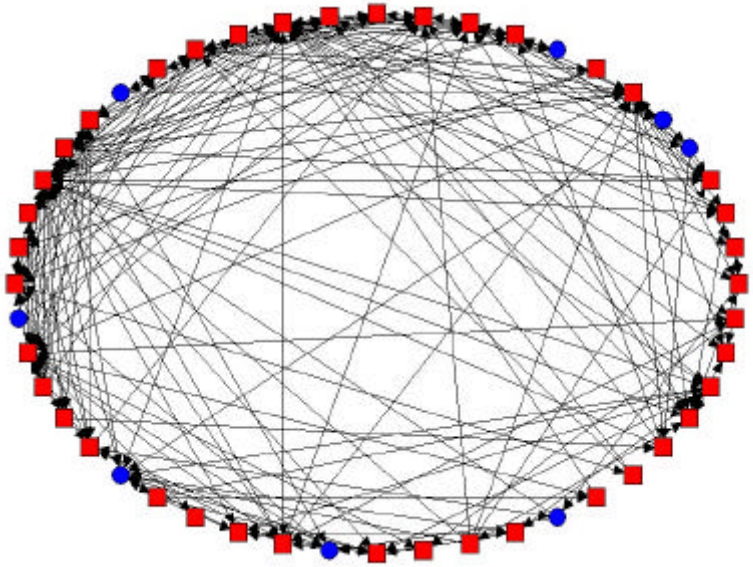
Collaboration ROLES - PHASE 3

Red squares=Math/Computer Sciences; Blue Circles=Applications



Collaboration ROLES - PHASE 4

Red squares=Math/Computer Sciences; Blue Circles=Applications



Collaboration Density:
Roles (Math/Computer Sciences versus Applications)

Phase 1

Members / Interviewees	Math/ CS	APPS
Math/ CS	.2778	.1111
APPS	.2778	1.000

Phase 2

Members / Interviewees	Math/ CS	APPS
Math/ CS	.3333	.2130
APPS	.1759	.1667

Phase 3

Members / Interviewees	Math/ CS	APPS
Math/ CS	.2047	.1255
APPS	.1822	.1410

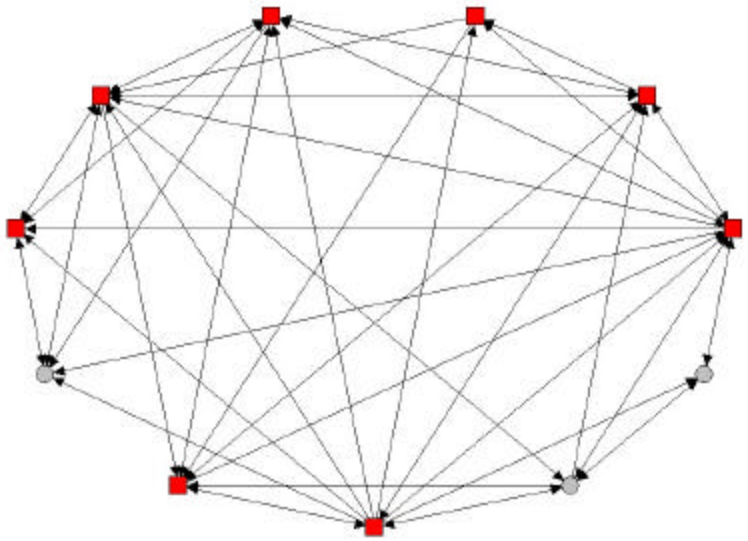
Phase 4

Members / Interviewees	Math/ CS	APPS
Math/ CS	.1503	.0656
APPS	.0723	.0536

CS = Computer Sciences APPS = Engineering/ Science Applications

Sources of Knowledge MICS – Phase 1

Red squares = MICS funding; Gray Circles= no MICS



Sources of Knowledge MICS – Phase 2

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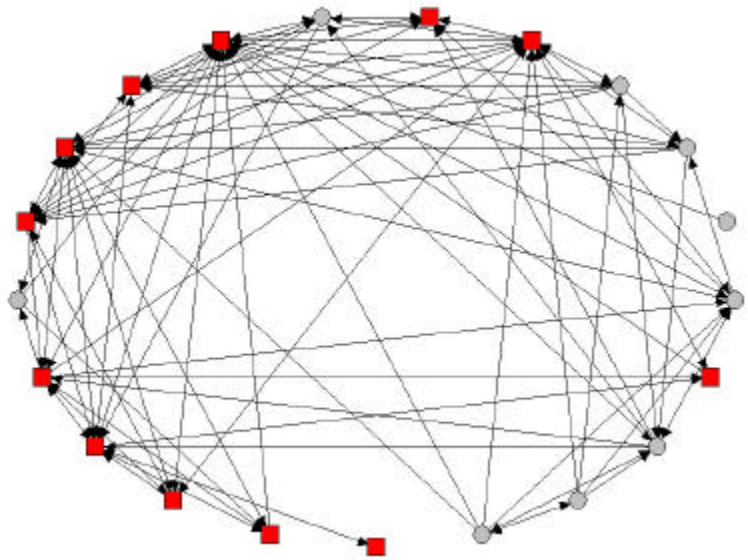

Sources of Knowledge MICS – Phase 3

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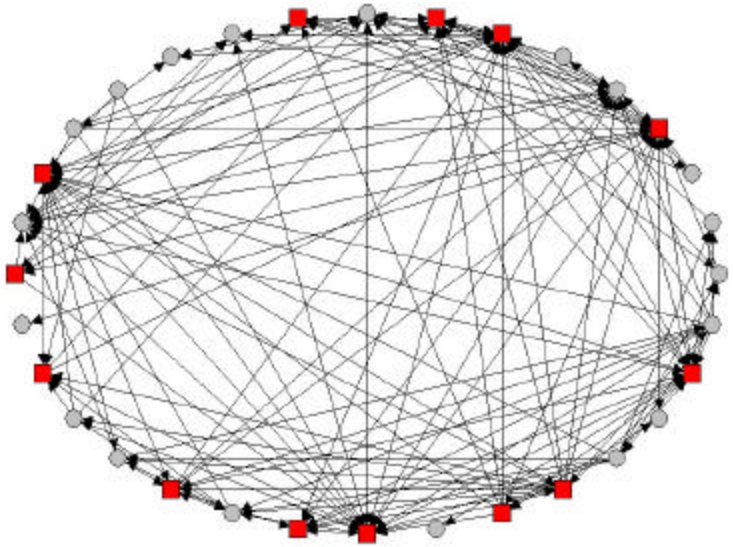

Sources of Knowledge MICS – Phase 4

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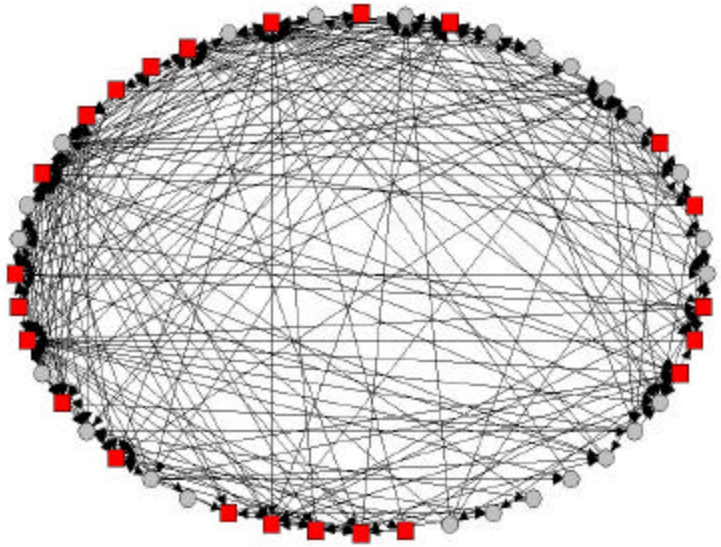


Sources of Knowledge: MICS versus Non-MICS Funding

Phase 1

Members / Interviewees	MICS	Non-MICS
MICS	.6071	.4167
Non-MICS	.2917	.3333

Phase 2

Members / Interviewees	MICS	Non-MICS
MICS	.4545	.1296
Non-MICS	.2500	.2083

Phase 3

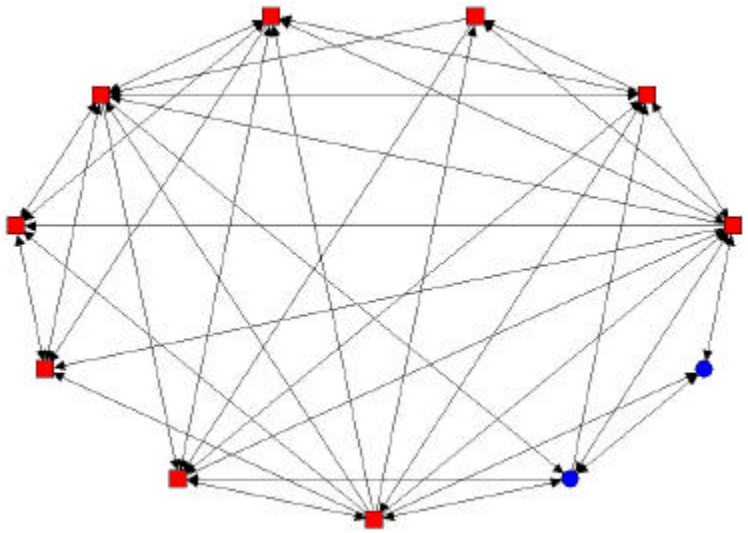
Members / Interviewees	MICS	Non-MICS
MICS	.4487	.1660
Non-MICS	.2470	.0819

Phase 4

Members / Interviewees	MICS	Non-MICS
MICS	.2410	.1530
Non-MICS	.1693	.0850

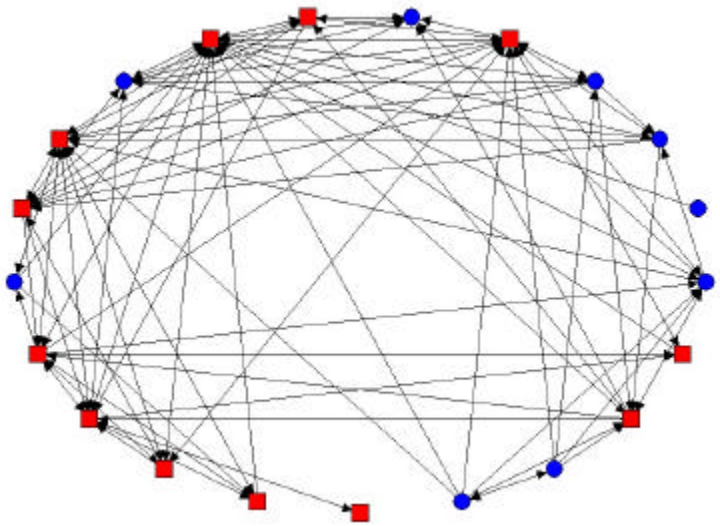
Sources of Knowledge ROLES – Phase 1

Red squares=Math/Computer Sciences; Blue Circles=Applications



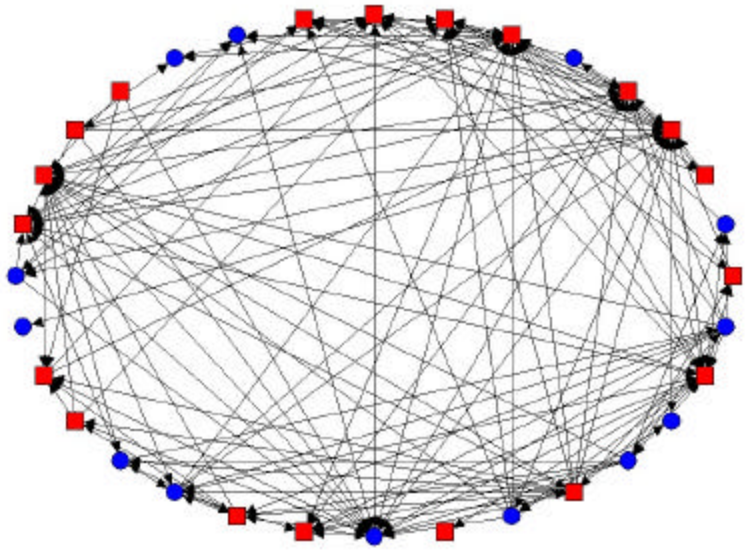
Sources of Knowledge ROLES – Phase 2

Red squares=Math/Computer Sciences; Blue Circles=Applications



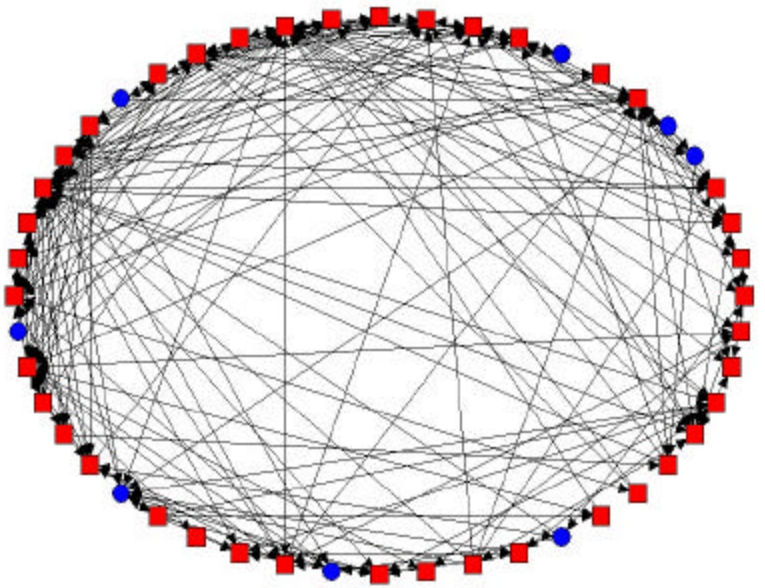
Sources of Knowledge ROLES – Phase 3

Red squares=Math/Computer Sciences; Blue Circles=Applications



Sources of Knowledge ROLES – Phase 4

Red squares=Math/Computer Sciences; Blue Circles=Applications



Sources of Knowledge:
Roles (Math/Computer Sciences versus Applications)

Phase 1

Members / Interviewees	Math/ CS	APPS
Math/ CS	.5694	.2778
APPS	.2778	1.000

Phase 2

Members / Interviewees	Math/ CS	APPS
Math/ CS	.4545	.1852
APPS	.2315	.1528

Phase 3

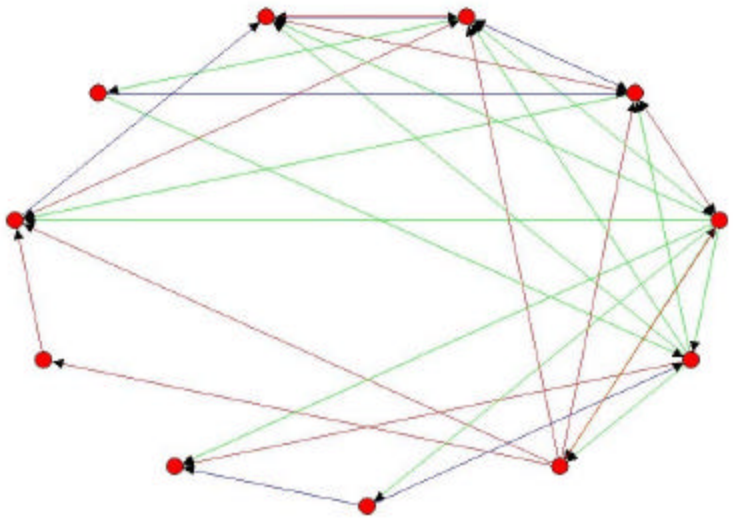
Members / Interviewees	Math/ CS	APPS
Math/ CS	.2807	.1457
APPS	.2065	.1090

Phase 4

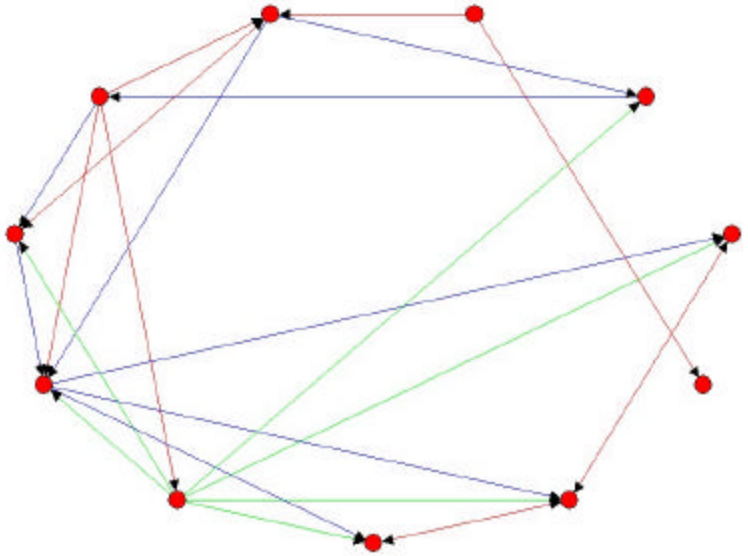
Members / Interviewees	Math/ CS	APPS
Math/ CS	.1897	.0875
APPS	.0943	.0714

CS = Computer Sciences APPS = Engineering/ Science Applications

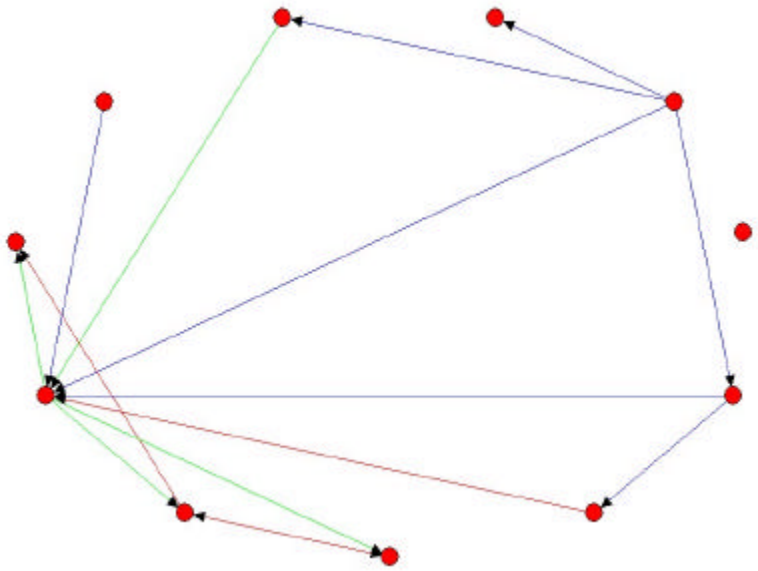
Sources of Knowledge – Phase 1
Mathematics Theoretical Knowledge
Red Line = Critical; Blue Line = Influential; Green Line = Helpful



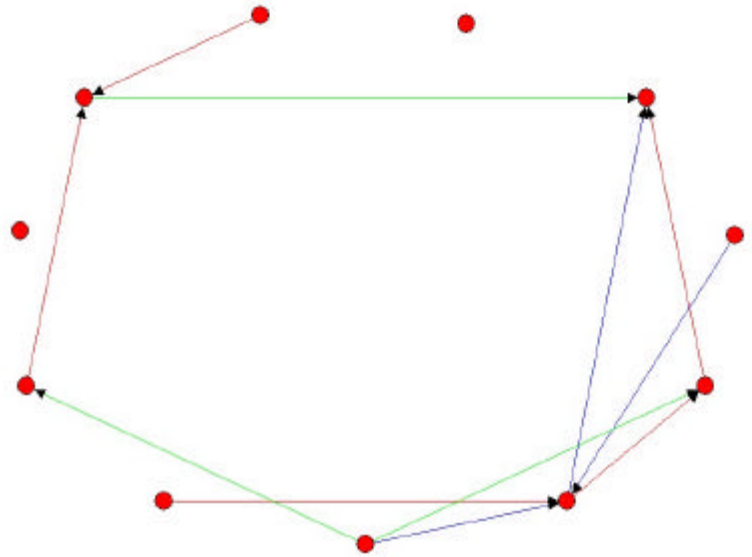
Sources of Knowledge – Phase 1
MPP Methodological Knowledge



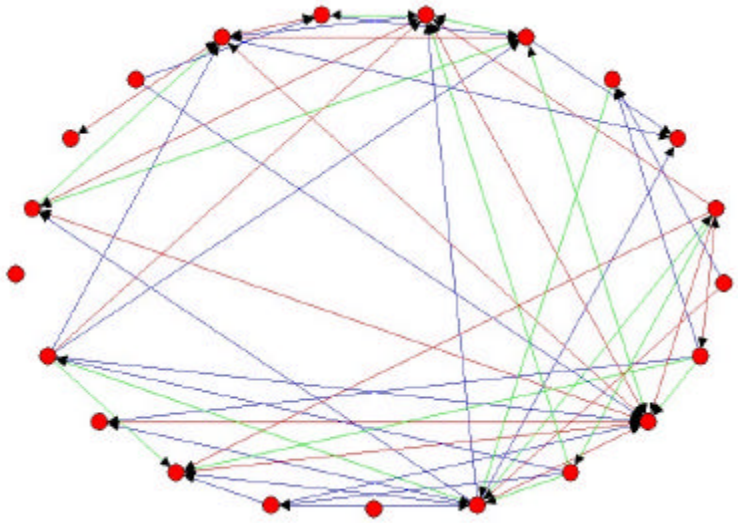
Sources of Knowledge – Phase 1
Knowledge from a Different Basic Discipline



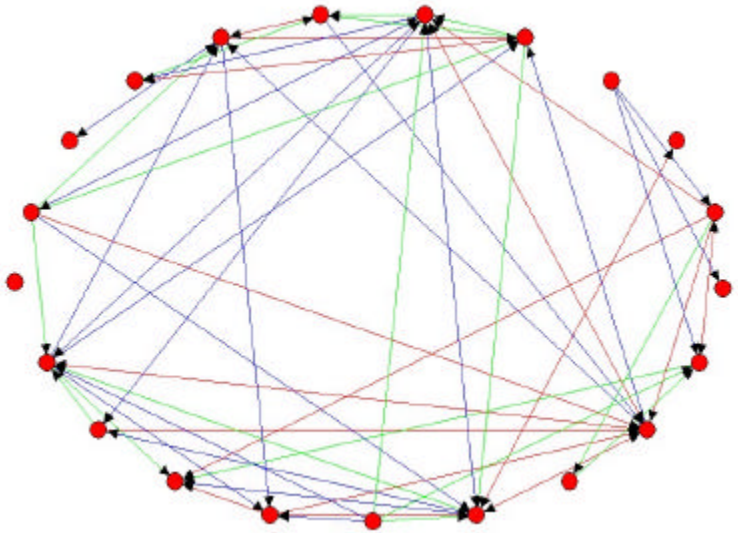
Sources of Knowledge – Phase 1
Knowledge About the Application



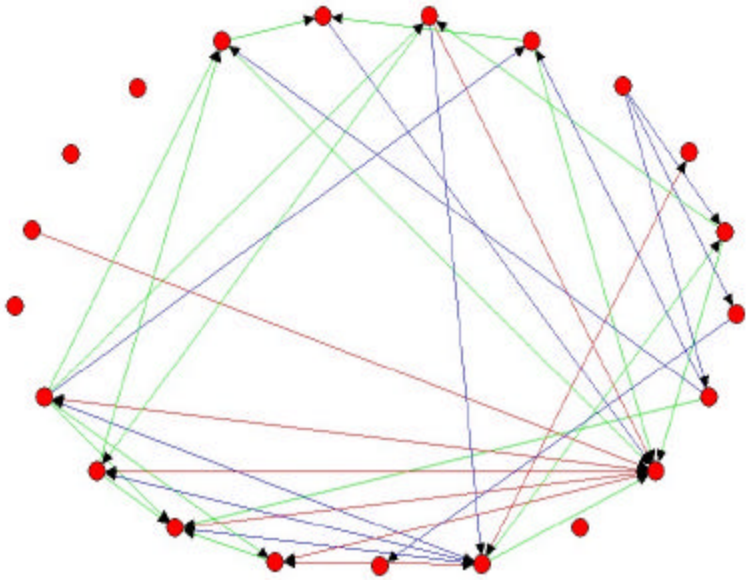
Sources of Knowledge – Phase 2
Mathematics Theoretical Knowledge
Red Line = Critical; Blue Line = Influential; Green Line = Helpful



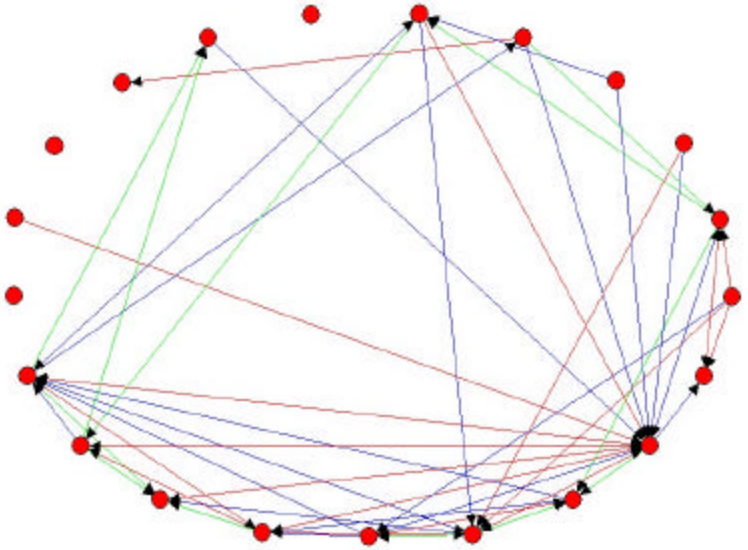
Sources of Knowledge – Phase 2
MPP Methodological Knowledge



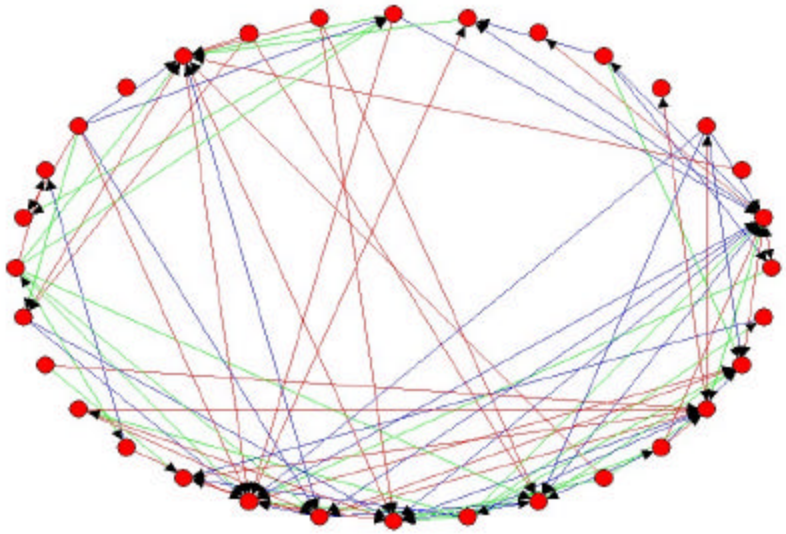
Sources of Knowledge – Phase 2
Knowledge from a Different Basic Discipline



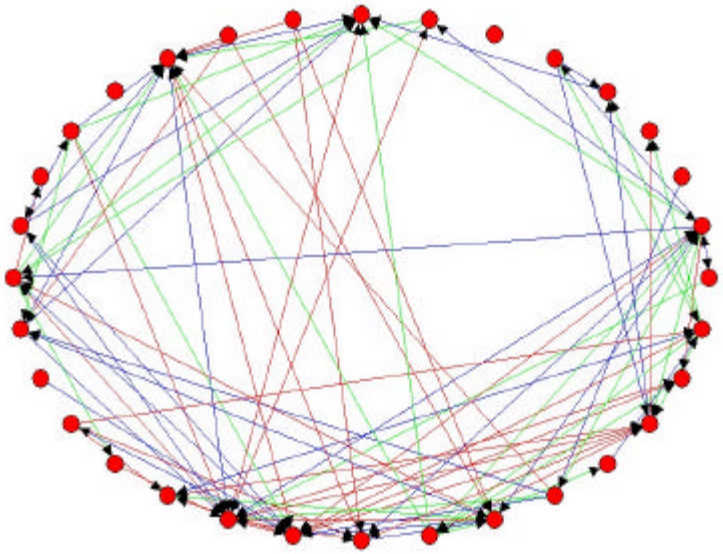
Sources of Knowledge – Phase 2
Knowledge About the Application



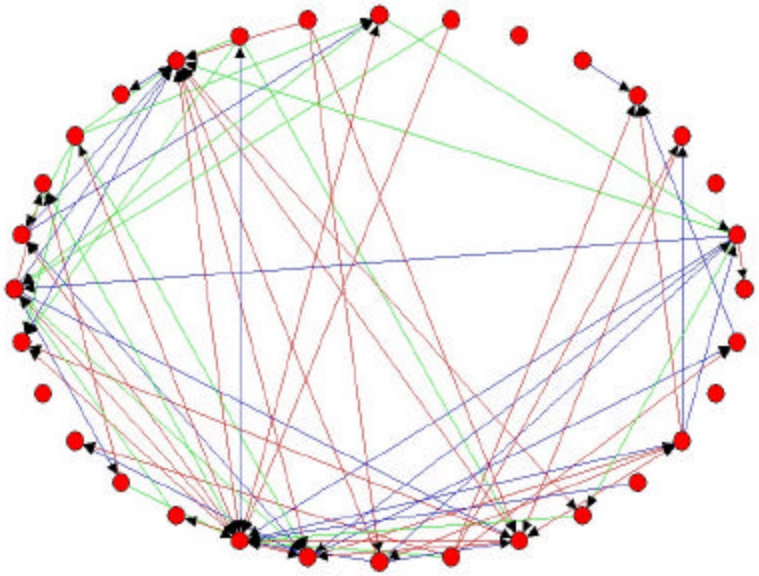
Sources of Knowledge – Phase 3
Mathematics Theoretical Knowledge
Red Line = Critical; Blue Line = Influential; Green Line = Helpful



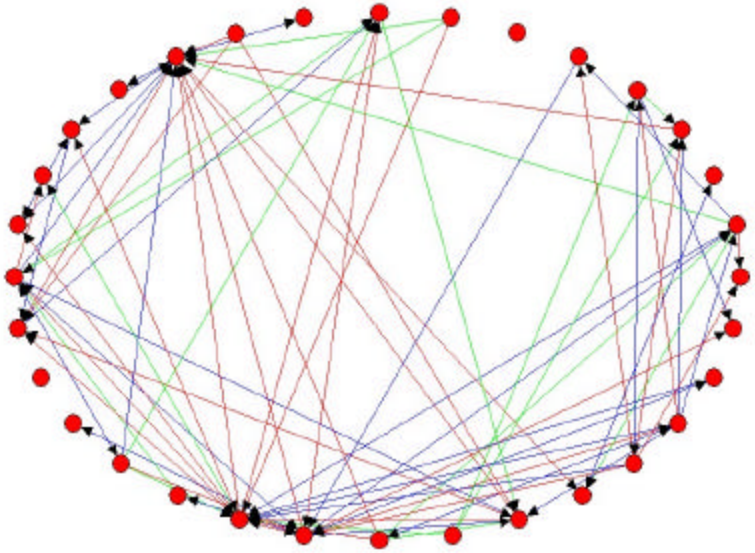
Sources of Knowledge – Phase 3
MPP Methodological Knowledge



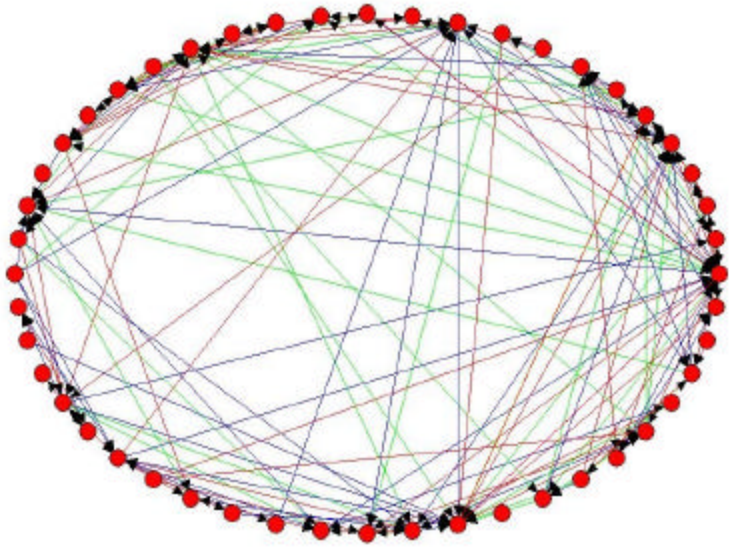
Sources of Knowledge – Phase 3
Knowledge from a Different Basic Discipline



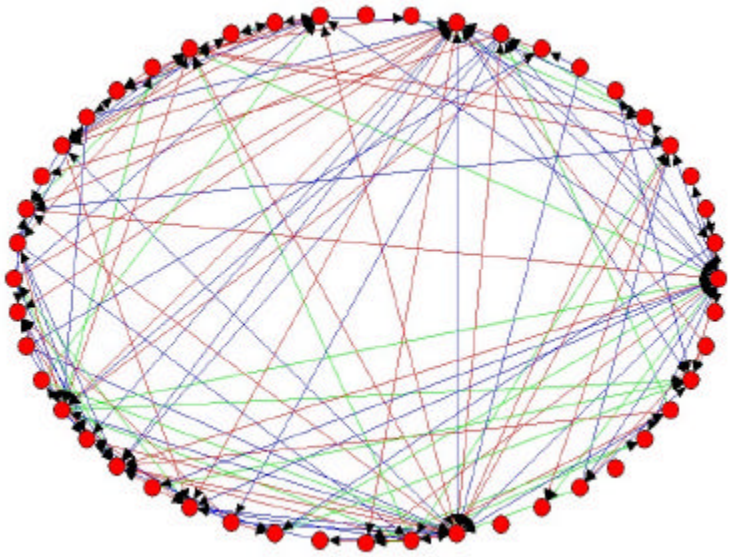
Sources of Knowledge – Phase 3
Knowledge About the Application



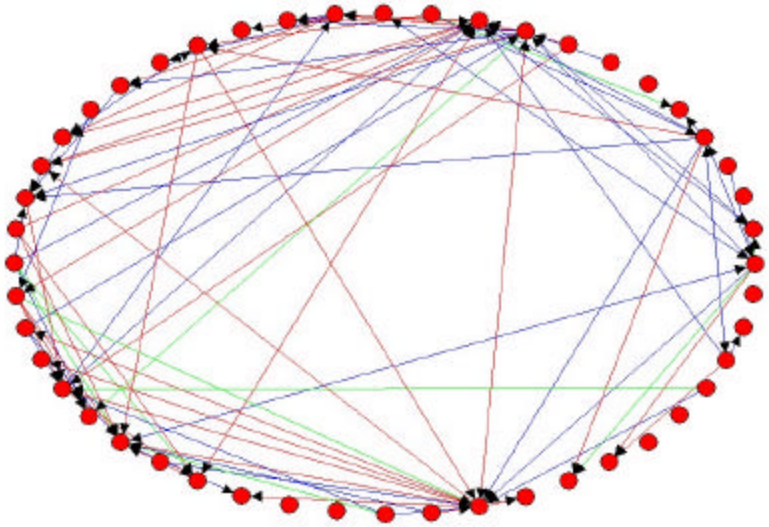
Sources of Knowledge – Phase 4
Mathematics Theoretical Knowledge
Red Line = Critical; Blue Line = Influential; Green Line = Helpful



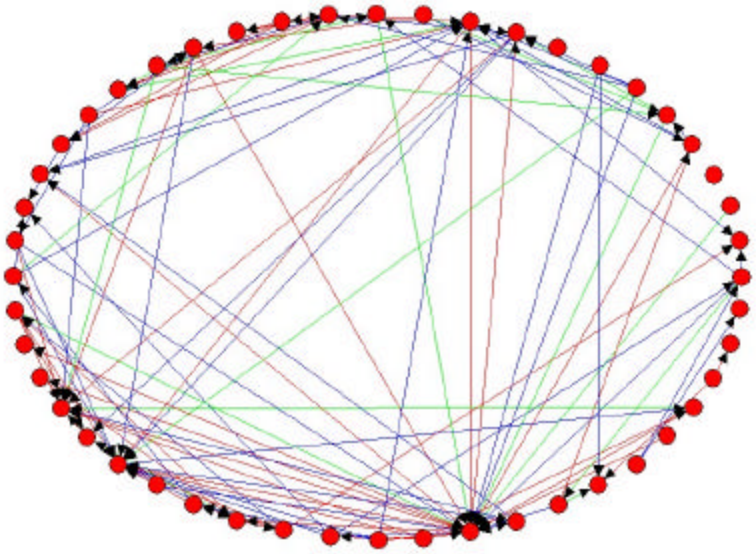
Sources of Knowledge – Phase 4
MPP Methodological Knowledge



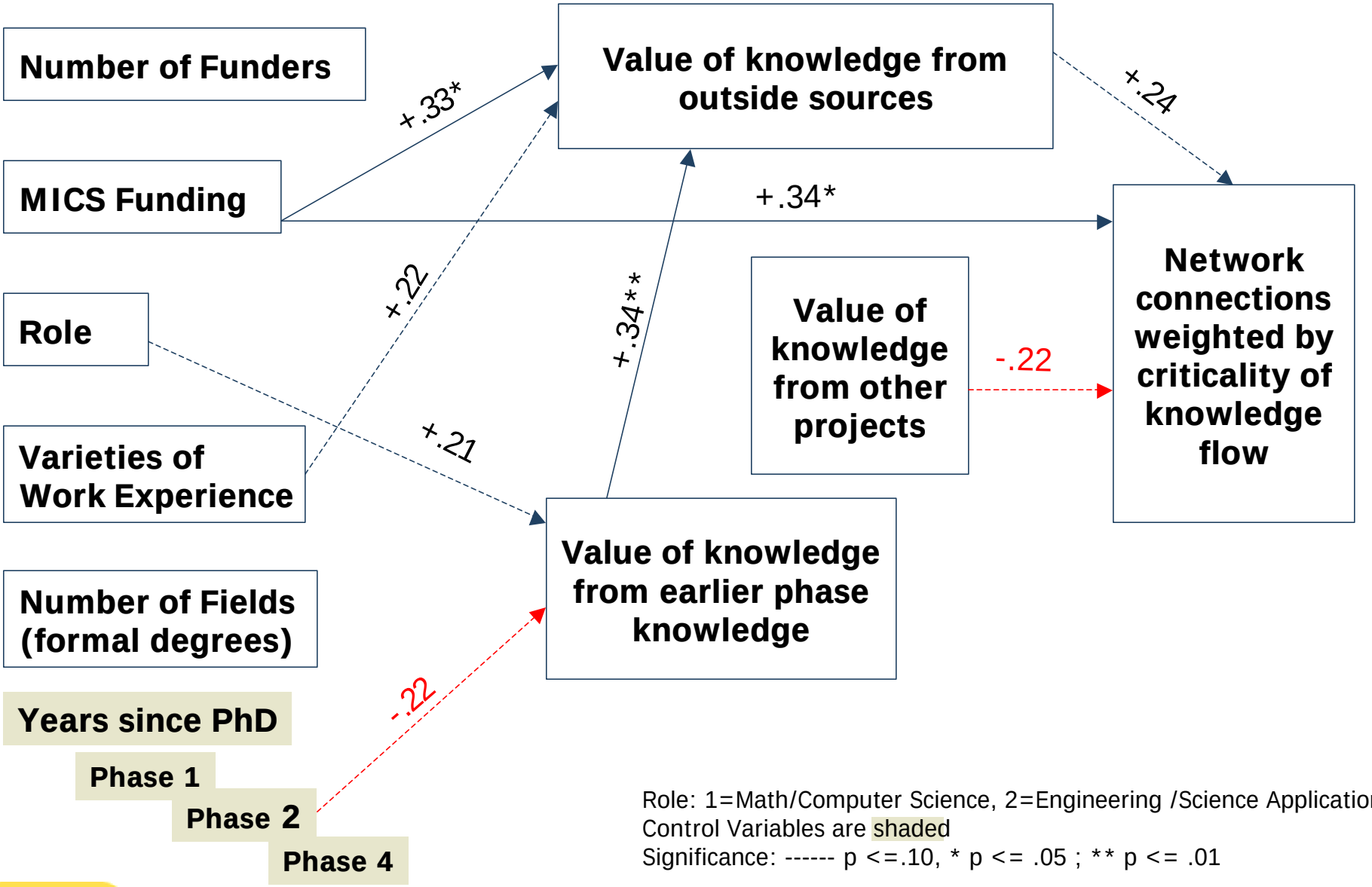
Sources of Knowledge – Phase 4
Knowledge from a Different Basic Discipline



Sources of Knowledge- Phase 4
Knowledge About the Application



Regression Path Diagrams to Total Network Connections Weighted by Criticality/Value of Knowledge Flow (In-Degree)



Role: 1=Math/Computer Science, 2=Engineering /Science Applications
Control Variables are shaded
Significance: ------ p <=.10, * p <= .05 ; ** p <= .01

Regressions – Outcomes Regressed on Network Knowledge Strength, Other Knowledge Sources, and Individual Researcher Attributes

Predictor Variables	Network Knowledge Strength	Strength of Contributions to MPP	Number of Math Articles	Number of Computer Science Articles	Number of Engineering / Science Articles
Controls[a]					
Phase 1	-.19	.11	**-.21***	**.44*****	.11
Phase 2	-.12	**.25***	-.07	.03	.02
Phase 4	-.07	-.18	.13	-.13	-.00
Age of Researcher's Ph.D.	.03	.07	**.17**[t]	.14	.11
Researcher Contributions					
Role (1= Math/Comp Sci, 2 = Apps)	-.07	**-.29****	**-.19***	-.04	**.44*****
MICS funding	**.34***	.09	**.25***	-.17	**-.25**[t]
Number of funding sources	-.04	.01	**.28****	.15	**.29***
Variety of past work experience	.10	**.27***	.14	.03	-.12
Number of degree fields	-.07	-.05	**-.27****	**.40****	**.40****
Knowledge Contributions [b]					
From earlier phases	.05	**.48*****	-.11	.06	-.04
From outside sources	**.24**[t]	.14	-.14	-.10	.02
From working on concurrent projects	**-.22**[t]	.14	.16	.06	-.05
Network Contribution					
Total Knowledge strength of network [c]	N/A	**.25***	**-.16**[t]	.17	**.40**
F	**1.90**	**5.32**	**6.60**	**3.07**	**3.20**
R^2	**.12***	**.42*****	**.48*****	**.26****	**.27****

[a] Phase 3 is the omitted phase dummy variable

[b] Sum of contributions/contributing sources, each weighted by the strength of its usefulness to researcher's work (1=helpful, 2=influential, 3=critical).

[c] Sum of weighted knowledge contributions by others in network plus intensity of knowledge sharing relationships with them.

Significance: *** $p \leq .001$
** $p \leq .01$
* $p \leq .05$
[t] $p \leq .10$

High Level Conclusions / Patterns Observed

- The Social Network Measures and Diagrams, the Qualitative Depiction of the Relationships, the Interactions, and Activities in the Network have a high degree of fit with each other.
- Examining the flows of knowledge into and through the social network appears promising as a way of predicting the knowledge outcomes.
- The nature of the collaborations that form and yield knowledge vary during the various phases of work that is carried out in the advancement of a particular area of knowledge.